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# Why are the $P_n$ and $S_n$ Methods Equivalent?

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## Introduction

I assume that the reader is familiar with the Spherical harmonics, $P_n$, method and the discrete ordinates, $S_n$, method; for a derivation of the equations used in these methods see the appendix. I will only discuss the Boltzmann equation in one dimension, and the $S_n$ method using Gaussian quadrature. I will do this merely to simplify the following discussion; once you understand the concepts presented here you can easily extend the conclusions to more general situations.

Why are the spherical harmonics $P_n$ and discrete ordinate $S_n$ methods, or more correctly the $P_n$ and $S_{n+1}$ methods, equivalent, e.g., $P_3$ is equivalent to $S_4$? When the $S_n$ method uses a Gaussian quadrature most textbooks will tell you that both methods are equivalent to assuming that the angular flux can be represented by a Legendre polynomial expansion of order n.

Most textbooks are wrong [1]! We know that the $S_n$ method constrains the "particles" to travel in discrete directions; when Gaussian quadrature is used these discrete directions correspond to the zeros of the Legendre polynomial $P_{n+1}(\mu)$. What is not immediately obvious is that the $P_n$ method constrains the "particles" in exactly the same way. That is why the two methods are equivalent. Let's discuss this in terms of physics and mathematics.

## Physical Argument

First let's look at this problem from a physical viewpoint. The standard $P_n$ method assumes that the (n+1)-th Legendre coefficient of a Legendre expansion of the angular flux is zero, at all spatial points, energies, and times; see the appendix for a derivation of the $P_n$ equations. This seems like an innocent enough assumption. But think about it:

physically how can the (n+1)-th Legendre coefficient of the angular flux be zero at all spatial points, energies, and times? The only way that this can occur is if the "particles" are constrained to travel only in discrete directions corresponding to the zeros of $P_{n+1}(\mu)$. Since the Legendre polynomials are a complete, orthogonal set, physically there is no other way that this can occur.

**Mathematical Argument**

Let's now look at this mathematically. Notice that above I didn't say that the $P_n$ method is equivalent to assuming that the angular flux is an n-th order polynomial; this is a common error made by many textbooks. All I said was that the (n+1)-th Legendre coefficient of a Legendre expansion of the angular flux is zero, at all spatial points, energies, and times. As we will see below, it is easy enough to prove that the $P_n$ method is NOT equivalent to assuming the flux is an n-th order polynomial. Assuming that the $P_n$ and $S_n$ methods are equivalent, let's see what this implies. I claim that the $P_n$ method is equivalent to assuming the angular flux is expressed as an infinite Legendre series, and the $S_n$ method models particles that stream in discrete directions. In which case if the two solutions are equivalent we have,

$P_n$ $S_{n+1}$

$$\sum_{j=0}^{\infty} \frac{2j+1}{2} P_j(\mu) F_j(Z) = \sum_{l=1}^{n+1} G_l(Z)\, \delta[\mu - \mu_l]$$

Multiplying by $P_k(\mu)$ and integrating over all directions we obtain a definition of an infinite number of Legendre coefficients, $F_k(Z)$, k = 0 to infinity, in terms of the n+1 $G_l(Z)$, l = 1 to (n+1), terms of the $S_n$ solution,

$$F_k(Z) = \sum_{l=1}^{n+1} G_l(Z) \int_{-1}^{+1} P_k(\mu)\, \delta[\mu - \mu_l]\, d\mu$$

$$F_k(Z) = \sum_{l=1}^{n+1} G_l(Z)\, P_k(\mu_l)$$

The first point to note is that since we are using Gaussian quadrature the discrete ordinates of the $S_n$ method, $\mu_l$, are the zeroes of $P_{n+1}$, so we can immediately see that the (n+1)-th Legendre coefficient of the $P_n$ solution, namely $F_{n+1}(Z)$, is exactly zero, which is what we assume for the $P_n$ method, so that this solution is of the form we expect,

$$F_{n+1}(Z) = \sum_{l=1}^{n+1} G_l(Z)\, P_{n+1}(\mu_l) = 0, \text{ because } P_{n+1}(\mu_l) = 0$$

The next point to note is that the higher order Legendre coefficients, for k=(n+2), (n+3),….to infinity, are generally not zero, so that the $P_n$ solution is not a polynomial of order n, but rather an infinite series, in which only the (n+1)-th Legendre coefficient is zero.

Another point to note is that the infinite series solution to the $P_n$ equations converges to the $S_{n+1}$ solution, and as such is equivalent to streaming in the discrete directions corresponding to the zeroes of the (n+1)-th Legendre polynomial.

We can also see that the higher order Legendre coefficients are not zero by examining the $P_n$ equations. These equations couple three successive Legendre moments of the angular flux, in the form, (see, the appendix for a derivation of this equation),

$$(k+1)*\lambda*F_{k+1}+k*\lambda*F_{k-1}+(2k+1)\Sigma tF_k=(2k+1)\Sigma s_kF_k$$

We close this set of equations by assuming that the (n+1)-th Legendre moments, $F_{n+1}$, is zero. We then end up with (n+1) equations in (n+1) unknowns, $F_k$, k = 0 to n, which we can solve.

What's not usually included in a description of the $P_n$ method is what the higher order equations tell us. For example, let's look at the above equaton with k = (n+1),

$$(n+2)*\lambda*F_{n+2}+(n+1)*\lambda*F_n+(2n+3)\Sigma tF_{n+1}=(2n+3)\Sigma s_{n+1}F_{n+1}$$

Since we assume that $F_{n+1}$ is zero, this equation tells us that $F_{n+2}$ is not zero, but rather that it is linearly dependent on $F_n$. So that once we solve the $P_n$ equations to define the Legendre moments of the flux, $F_k$, k = 0 to n, we can use $F_n$ to define $F_{n+2}$. We can continue in this manner to define all of the higher order Legendre moments toward n = infinity.

In general, since the $P_n$ equations couple three successive Legendre moments if we assume any two successive moments are exactly zero, then we must conclude that the same is true of the third. This would allow us to march in increasing order n, upward from the n-th equation to prove that all higher order moments are zero. However, it would also allow us to march in decreasing order n, downward from the n-th equation to prove that all lower order moments, including the scalar flux, $F_0(Z)$ is exactly zero. This leads to the nonsense conclusion that the only possible solution is zero. Therefore we must conclude that two successive moments cannot be zero.

This conclusion can be generalized even further by realizing that no two Legendre polynomials of different order n, have the same zeroes, except for the trivial case, $\mu = 0$. Therefore our definition of the infinite series of Legendre moments in terms of the $S_n$ solution,

$$F_k(Z) = \sum_{l=1}^{n+1} G_l(Z)\ P_k(\mu_l)$$

tells us that in general all of the Legendre moments, except for (n+1), are non-zero.

**So What?**

Generally if the $P_n$ or $S_n$ methods are used only to define the lower order moments of the flux, such as the scalar flux and current, the fact that both methods correspond to streaming in discrete directions will have little impact on your results, and for a wide class of applications you can obtain accurate answers for these lower order moments. Therefore for these applications there is no problem in your interpretation of the results.

This is because the proper way to interpret the $P_n$ and $S_n$ solutions is not in a continuous sense as a function of direction, but rather in an integral sense. For example, Gaussian quadrature can accurately define the integral of polynomials. Note, I said the integral effect of polynomials, not necessarily the continuous polynomials themselves. So that the $S_n$, and the equivalent $P_n$ method, can accurately define the lower order moments of our angular distribution, such as the scalar flux and current, which in many applications is all that we are interested in.

However, a problem can occur if you assume that the $P_n$ solution is an n-th order polynomial that can be used to define the angular flux as a continuous function of direction; as you can see from the above, this is not true, even though most textbooks say that it is true. Again, let me repeat: the $P_n$ solution is an infinite Legendre series in which only the (n+1)-th Legendre moment is zero, and this series converges to streaming in discrete directions, corresponding to the zeroes of $P_{n+1}(\mu)$. As such this solution does not directly define the continuous angular distribution of the flux. Failure to realize this can lead to inaccurate results, e.g., there is no guarantee that the sum of the first (n+1) terms of the Legendre series is everywhere positive, and as such it is chancy to assume that this is a good approximation to the actual angular distribution.

**Improving our Discrete Ordinate Method**

Once you accept the equivalence between the $P_n$ and $S_n$ methods you can use this equivalence to good advantage. You can use the best features of each method to improve the methods you use. For example, in the $P_n$ method most time is spent finding the eigenvalues; once they are defined it is merely a matter of matching boundary conditions. In contrast, in the $S_n$ method most time is spent iterating between spatial points, along the characteristic directions. As a result, in terms of speed, $P_n$ works well in optically thick spatial regions where we need only be concerned with matching boundary conditions, and $S_n$ converges fastest in optically thin spatial zones where not too many spatial points are required. So that you can use the two methods in combination to accelerate your calculations.

As another example of what we can learn from the equivalence between these two methods, consider the relationship between the Legendre moments from the $P_n$ method and the discrete weights from the $S_n$ method,

$$F_k(Z) = \sum_{l=1}^{n+1} P_k(\mu_l) G_l(Z)$$

But we also know that the $P_n$ solution is a sum of exponentials,

$$F_k(Z) = \sum_{m=0}^{n} F_{km}\, e^{\lambda m * Z}$$

Where the eigenvalues $\lambda_m$ depend on the multiplication of the system, and the coefficients $F_{km}$ depend on the boundary conditions.

This in turns tells us the form of the $S_n$ solution that we should expect,

$$\sum_{m=0}^{n} F_{km}\, e^{\lambda m * Z} = \sum_{l=1}^{n+1} P_k(\mu) G_l(Z)$$

Above I said that the $P_n$ and $S_n$ methods are equivalent. This is true only up to the point where the $S_n$ method introduces an additional assumption by expanding the flux in space; see the appendix for a derivation of the $S_n$ equations. This additional step breaks the exact equivalence between the two methods, and can lead to non-physical results, such as oscillating or even negative flux, in $S_n$ calculations.

The $S_n$ method is not the only discrete ordinate method available to us. Based upon the above equivalence between the $P_n$ solution, that we know is a sum of exponentials in space, and the $S_n$ solution, suggests that rather than using the most common $S_n$ assumption that the flux is linear in space, it would be better to assume exponential variation. This is what the NIOBE method [Numerical Integration Of the Boltzmann Equation] does; this method was developed circa 1960 by the United Nuclear Corp. [2], but was somehow forgotten when the $S_n$ method came into vogue.

Let me illustrate in the simplest case: planar geometry with isotropic scattering; see the appendix for details,

$$\mu \frac{\partial N}{\partial Z} + \Sigma t N = \frac{\Sigma s N0}{2}$$

$$\mu \frac{\partial}{\partial Z}\{N \exp[\Sigma t Z/\mu]\} = \frac{\Sigma s N0}{2} \exp[\Sigma t Z/\mu]$$

$$N(Z2,\mu) = N(Z1,\mu)\exp[-\Sigma t(Z2-Z1)/\mu] + \frac{1}{2\mu}\int_{Z1}^{Z2} \Sigma s(Z')N0(Z')\exp[-\Sigma t(Z2-Z')/\mu]dZ'$$

In this form we find that,

1) If you use any method to accurately define the scalar flux, $N_0(Z)$, you can define the angular flux as a line integral, starting from your known boundary condition

and methodically working your way through your geometry. That's essentially all a discrete ordinate method does, except in the above equation you are not constrained to a given set of discrete ordinates, i.e., you can define the angular distribution in as many directions as you need.

2) In order to do this you need only explicitly introduce an approximation for the scalar flux, $N_0(Z)$, but not the angular flux, which in the above equation only appears at discrete spatial points, Z1 and Z2.
3) For a discrete ordinate method the above equations can be used to illustrate the NIOBE method in which exponential, rather than linear, variation of the scalar flux, $N_0(Z)$ is assumed. The resulting algorithm is stable and if you start from non-negative boundary conditions to initialize your iteration, you will find that unlike the $S_n$ method, you cannot end up with non-physical, negative flux.
4) Since there are so many $S_n$ codes available, what's nice about the NIOBE method is that it is so similar to the $S_n$ method that it is fairly easy to modify an existing $S_n$ code to use the NIOBE method.
5) Above I've only discussed isotropic scattering in planar geometry. This was done only to simplify notation; once you understand the NIOBE concept you can generalize to anisotropic scattering in more complicated geometry, e.g., the NIOBE method is so similar to the $S_n$ method that any geometry that $S_n$ can handle, can be handled by NIOBE.

**Conclusions**

It has been shown that both the $P_n$ and $S_n$ methods constrain the "particles" to stream in discrete directions. In particular it has been shown that contrary to what it says in most textbooks, the $P_n$ solution is not an n-th order polynomial; rather it is an infinite series of Legendre polynomials, in which only one of the Legendre coefficients is zero, and the series converges to the same streaming in discrete directions that is used in the $S_n$ method. This is why the two methods are equivalent.

This conclusion means that you should not assume that the $P_n$ solution is an n-th order polynomial that can be used to accurately define the angular distribution. If you do need to define the angular distribution, I suggest you consider using the above defined line integral using the previously calculated lower order Legendre moments of the flux.

Realizing the equivalence between these two methods has the potential to improve how our discrete ordinate methods are used, and how to define an angular flux.

**References**

[1] There are so many textbooks that make the wrong assumption about the spherical harmonics, $P_n$, method, that it does not seem fair for me to reference any one textbook to illustrate this error.

[2] "A program for the Numerical Integration of the Boltzmann Transport Equation – Niobe," by S. Preiser, ARL 60-314 (Dec. 1960).

## Appendix

### Derivation of the Spherical Harmonics, $P_n$, Equations

In order to simplify the notation and equations, I will derive the $P_n$ equations in planar geometry, for the time independent case,

$$\mu \frac{\partial F(Z,\mu)}{\partial Z} + \Sigma t F(Z,\mu) = \frac{1}{2} \sum_{l=0}^{L} \quad \Sigma s_l F_l(Z) P_l(\mu)$$

Multiply by the Legendre polynomial, $(2n+1)P_n(\mu)$, and use the relationship between Legendre polynomials of varying orders,

$$(2n+1)\mu * P_n(\mu) = (n+1)P_{n+1}(\mu) + nP_{n-1}(\mu)$$

to obtain the $P_n$ equations, that define the coupling between any three successive moments of the angular flux,

$$(n+1)\frac{\partial F_{n+1}(Z)}{\partial Z} + n\frac{\partial F_{n-1}(Z)}{\partial Z} + (2n+1)\Sigma t F_n(Z) = (2n+1)\Sigma s n F_n(Z)$$

The infinite set of equations is closed by assuming that $F_{n+1}(Z)$ is zero; this gives us (n+1) equations, in (n+1) unknowns, $F_k$, k=0 to n. It is well known that the solution of these equations is the sum of a series of discrete eigenvalues, so we can assume,

$$F_n(Z) = F_n * Exp[\lambda * z]$$

and the equations become,

$$(n+1) * \lambda * F_{n+1} + n * \lambda * F_{n-1} + (2n+1)\Sigma t F_n = (2n+1)\Sigma s n F_n$$

This is an eigenvalue problem where we must solve for the set of discrete eigenvalues, $\lambda$, and the coefficients $F_n$ are then defined to match boundary conditions.

### Derivation of the discrete Ordinate, $S_n$ Equations

I will derive the $S_N$ equations for exactly the same situation as I used above to derive the $P_n$ equations; namely planar geometry, for the time independent case,

$$\mu \frac{\partial F(Z,\mu)}{\partial Z} + \Sigma t F(Z,\mu) = \frac{1}{2} \sum_{l=0}^{L} \quad \Sigma s \;\; P_l(\mu)\, F_l(Z)$$

where the Legendre moments of the flux are defined by quadrature,

$$F_l(Z) = \sum_{n=1}^{N} F(Z, \mu n)\, w_n$$

We will solve the above equation using N discrete directions for $\mu$,

$$\mu k \frac{\partial F(Z,\mu k)}{\partial Z} + \Sigma t F(Z,\mu k) = \frac{1}{2}\sum_{l=0}^{L} \Sigma s\ P_l(\mu k) \sum_{n=1}^{N} F(Z,\mu n)\, w_n,\ k = 1 \text{ to } N$$

Integrating over a spatial interval Z1 to Z2

$$\mu k\{F(Z2,\mu k) - F(Z1,\mu k)\} + \int_{Z1}^{Z2} \Sigma t F(Z,\mu k)\, dZ =$$
$$\frac{1}{2}\sum_{l=0}^{L} P_l(\mu k) \sum_{n=1}^{N} w_n \int_{Z1}^{Z2} \Sigma s\ F(Z,\mu n)\, dZ$$

Defining,

F(j+1/2,k) = F(Z2, $\mu k$) [cell edge flux]
F(j-1/2,k) = F(Z1, $\mu k$) [cell edge flux]
F(j ,k) = $\frac{1}{h}\int_{Z1}^{Z2} F(Z,\mu k)\, dZ$ [cell average flux]

$$\mu k\{F(j+1/2,k) - F(j-1/2,k)\} + <\Sigma t> h * F(j,k) =$$
$$\frac{1}{2}\sum_{l=0}^{L} P_l(\mu k) \sum_{n=1}^{N} w_n <\Sigma s>\ h * F(j,n)$$

To solve these equation we assume a relationship between cell average flux and cell average fluxes. The most common assumption is the "diamond difference" scheme, where the cell average flux is assumed to be equal to the average of the cell edge fluxes, e.g.,

$$F(j,k) = \frac{1}{2}\{F(j+1/2,k) + F(j-1/2,k)\}$$

which is equivalent to assuming linear interpolation of the angular flux.

**Derivation of the NIOBE Equations**

I will derive the NIOBE equations for exactly the same situation as I used above to derive the $P_n$ equations; namely planar geometry, for the time independent case,

$$\mu \frac{\partial F(Z,\mu)}{\partial Z} + \Sigma t F(Z,\mu) = \frac{1}{2} \sum_{l=0}^{L} \quad \Sigma s \, F_l(Z) P_l(\mu)$$

We can write this in a simpler form by multiplying by $\exp[\Sigma t Z / \mu]$ and combining the two terms on the left hand side of our equation, to find,

$$\mu \frac{\partial}{\partial Z} \{F \exp[\Sigma t Z / \mu]\} = \frac{1}{2} \exp[\Sigma t Z / \mu] \sum_{l=0}^{L} \quad \Sigma s \; F_l(Z) P_l(\mu)$$

which we can immediately integrate between any two space points Z1 and Z2, to find,

$$F(Z2,\mu) = F(Z1,\mu) \exp[-\Sigma t (Z2 - Z1)/\mu] +$$
$$\frac{1}{2\mu} \sum_{l=0}^{L} \quad P_l(\mu) \int_{Z1}^{Z2} \quad \Sigma s \, F_l(Z') \exp[-\Sigma t \, (Z2 - Z')/\mu \;] dZ'$$

In order to solve these equations the only approximation that we have to explicitly introduce is an approximation for the spatial variation of the Legendre moments of the flux. In particular note that we do not have to explicitly introduce any approximation for the spatial variation of the angular flux, $F(Z, \mu)$, since this only appears in the above equation at discrete space points Z1 and Z2.

For example, in the simplest case with isotropic scattering, in order to solve these equations for the angular flux, $F(Z, \mu)$, we only have to explicitly introduce an approximation for the scalar flux, $F_0(Z)$.

Here we are free to introduce any approximation for the Legendre moments, as long as our approximation is consistent with the derived angular flux at the discrete space points Z1 and Z2. For example, for the angular distribution at any given space point we could use the same quadrature approach as that used by the $S_n$ method, or we could assume the angular distribution is piecewise continuous; there are any number of physically acceptable assumptions that can be used. Similarly for the spatial variation of the Legendre moments of the flux, we could the same most common linear assumption used by the $S_n$ method, or we could assume exponential variation; again, there are any number of physically acceptable assumptions that can be used.

**Derivation of the Case's Method**

I will derive Case's method for exactly the same situation as I used above to derive the $P_n$ equations; namely planar geometry, for the time independent case,

$$\mu \frac{\partial F(Z,\mu)}{\partial Z} + \Sigma t F(Z,\mu) = \frac{1}{2} \sum_{l=0}^{L} \quad \Sigma s \, F_l(Z) P_l(\mu)$$

Assuming exponential variation.

$$F(Z,\mu) = F(\mu) * Exp[Z/\nu]$$

$$\mu * F(\mu) + \nu * \Sigma t F(\mu) = \frac{\nu}{2} \sum_{l=0}^{L} \Sigma s \, F_l P_l(\mu)$$

$$F(\mu) = \frac{\nu}{2[\mu + \nu * \Sigma t]} \sum_{l=0}^{L} \Sigma s \, F_l P_l(\mu)$$

Which defines the angular distribution, $F(\mu)$, directly in terms of its Legendre moments, $F_l$. Multiplying by $P_k(\mu)$ and integrating over $\mu$ we define the Legendre moment,

$$Fk = \frac{\nu * \Sigma s}{2} \sum_{l=0}^{L} F_l \int_{-1}^{+1} \frac{d\mu}{2[\mu + \nu * \Sigma t]} P_l(\mu) P_k(\mu)$$

In general this is a coupled set of transcendental equations defining the eigenvalues $\nu$. In the simplest case of isotropic scattering we have,

$$F_0 = \frac{\nu * \Sigma s}{2} F_0 \int_{-1}^{+1} \frac{d\mu}{2[\mu + \nu * \Sigma t]}$$

$$1 = \frac{\nu * c}{2} \mathrm{Ln}\left[\frac{1+\nu}{1-\nu}\right], \; c = \frac{\Sigma s}{\Sigma t}$$

In this case the solution is a single pair of discrete eigenvalues, $+/-\nu_0$, plus a continuum for $\nu$ between –1 and +1,

$$F(Z,\mu) = A[+\nu_0] \; Exp[Z/\nu_0] + A[-\nu_0] \; Exp[-Z/\nu_0] + \int_{-1}^{+1} A[\nu] Exp[Z/\nu] d\nu$$

Case's "solution" is really just a transformation of the original differential equation into an integral form, that can be just as difficult to solve as the original form. However, what this approach tells us is the eigenvalues; particularly the discrete eigenvalues. When you use any of the above described methods you are approximating these eigenvalues, and the accuracy of your approximation depends both on the order of the method that you use [e.g., $S_N$, where N is the order] and the quadrature used [above I've only discussed Gaussian quadrature, but we could use a different quadrature]. I'll merely mention here that one option that you have is to define your quadrature to reproduce the discrete eigenvalues of your system, as defined by Case's method.

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